Supplementary Information: Activity-Induced Stiffness, Entanglement Network and Dynamic Slowdown in Unentangled Semidilute Polymer Solutions

Jing Li, Bokai Zhang,^{*} and Zhi-Yong Wang[†] School of Physical Science and Technology, Southwest University, Chongqing 400715, China and Chongqing Key Laboratory of Micro-Nano Structure Optoelectronics, Chongqing 400715, China

I. Time evolution conformational function

The deviation function χ and the end-to-end distance as a function of time are presented in Figure S1 at different activity differences. The values of χ and R_e reach maximum at about $t_{max} = 1.5 \times 10^4 \tau$. At large activity difference, a decay in the two functions is observed,



FIG. S1: The time evolution of deviation function (a) and the end-to-end distance (b) at $\rho_m = 0.1$ for various activity differences. Shade is standard deviation.



FIG. S2: The time evolution of deviation function (a) and the end-to-end distance (b) at low density $\rho_m = 0.014$ for activity difference $\Delta T = 8$. Shade is standard deviation.

^{*} zbk329@swu.edu.cn

 $^{^\}dagger$ zywang@swu.edu.cn

resulting from interchain interaction exerted by the surrounding chains. In low density, $\rho_m = 0.014\sigma^{-3}$, the decay is not observed as shown in Figure S2. The average end-to-end distance results are obtained by calculating the mean of the data during the steady state.

II. Effective stiffness

Here, we used different static quantities to describe the effective stiffness at local bond length scale (bond angle distribution), at large chain length scale (single-chain structure factors and mean-square internal distance).

A. Bond angles

In the system of active polymers, the distributions of bond angles in Figure S3a are almost identical for different activity differences. For passive system of SPCs, the change in bond angle distribution and the mean bond angles are significant with the increase of local bending energy. In addition, the persistent lengths extracted from the bond-bond correlation functions (see Figure S4a) increase more dramatically in SPCs as shown in Figure 2 of maintext.



FIG. S3: (a) Bond angle distribution of active polymers at various activity differences. (b) Bond angle distribution of SPCs at various bending energy coefficients. (c) The mean angles as a function of activity difference (the blue *x*-axis on the bottom) and bending energy coefficient (the red *x*-axis on the top).



FIG. S4: (a) Bond angle correlation of SPCs as a function of contour distance. (b) Single-chain structure factor of SPCs.

B. Single-chain structure factors

The single-chain structure factor describes density fluctuation of monomers for the same chain at length scale $\sim 2\pi/q$, and it is defined as

$$\omega(q) = \frac{1}{N} \sum_{i,j}^{N} \langle exp[-i\boldsymbol{q}(\boldsymbol{r}_{i}^{a} - \boldsymbol{r}_{j}^{a})] \rangle$$
(1)

where \mathbf{r}_i^a is the position vector of *i*-th monomer belonging to *a*-th chain, $\langle ... \rangle$ denotes spatial isotropic average and the statistical average across multiple chains and ensembles.

For SPCs systems, the single-chain structure factor exhibits minimal variation with bending energy, suggesting that the local bending energy has limited impact at intermediate scales.

III. Radial distribution function

We calculated the radial distribution function of monomers that belong to different chains. Figure S5 shows that $g_{mm}(r)$ increases with activity difference, indicating enhanced interchain interactions, which aligns with the observed average adsorption number $\langle n \rangle$.



FIG. S5: Radial distribution function of interchain monomers for active polymers (a) and SPCs (b).



FIG. S6: The center-of-mass mean-square displacement of active polymers (a) and SPCs (c). The Rouse mode autocorrelation function of active polymers (c) and SPCs (d).

V. Effective temperature

Figure S7 shows the velocity distributions of hot monomers on the terminals and cold monomers on the center in active polymers, which conform to Maxwell's velocity distribution, $P_{Maxwell}(v)$. The velocity distribution function can be used to obtain the mean-square velocity on hot or cold monomers through $\bar{v}^2 = \int_0^\infty P(v)v^2dv$. The effective temperature can be obtained by utilizing the energy equipartition theorem, $\frac{3}{2}k_BT_{eff} = \frac{1}{2}m\bar{v}^2$.



FIG. S7: Velocity distributions of hot monomers and cold monomers in active polymers. The lines represent the fitting to Maxwell's velocity distribution.